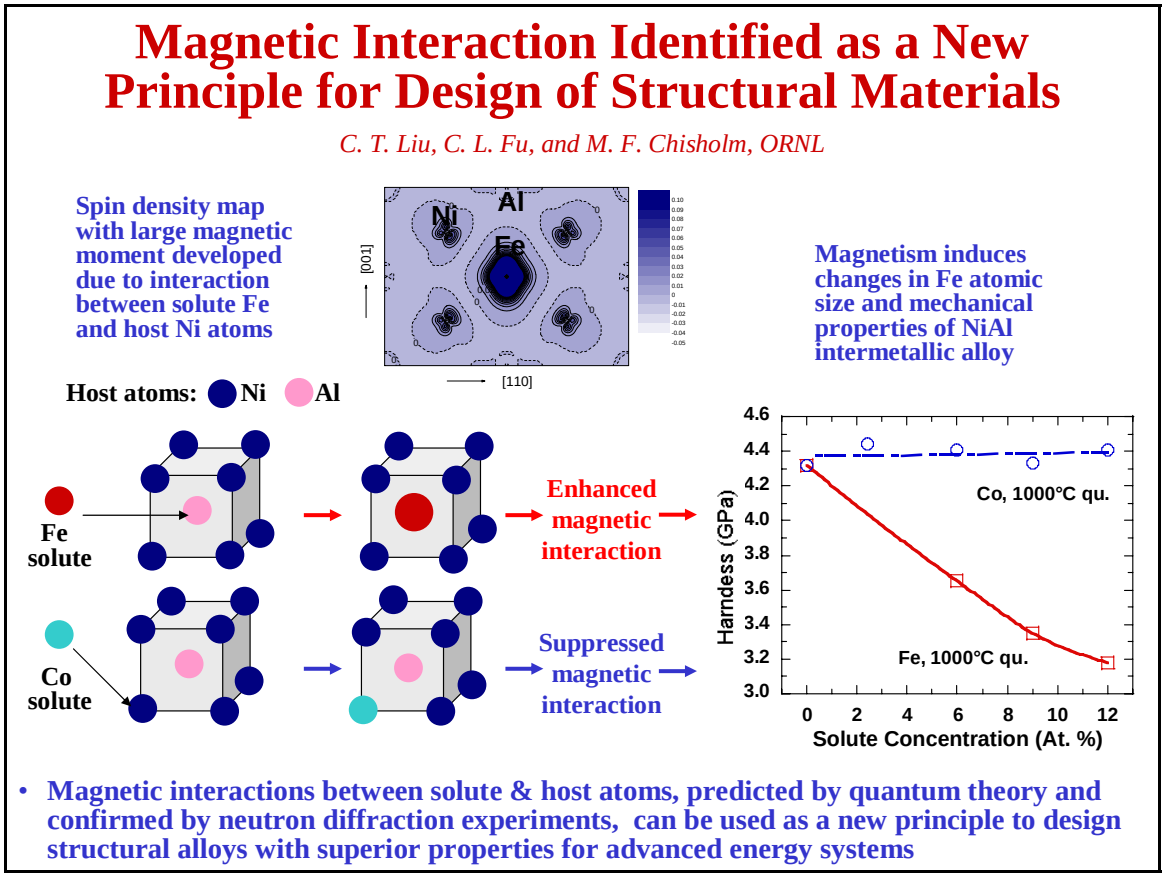
Mechanical Properties Affected by Magnetic Interaction: A New Fundamental Principle

Investigators: C. T. Liu, C. L. Fu, and M. F. Chisholm, ORNL

Quantum effects involving magnetic interaction have been discovered to be responsible for unexpected solid solution hardening/softening in intermetallic alloys, thus resulting in their superior mechanical properties. This new phenomenon was discovered by careful coordination between theory and experiments: first-principle quantum-mechanical calculations coupled with polarized neutron diffraction and electron energy-loss spectroscopy (EELS). Experimental studies have revealed unusual interatomic spacing and resultant solid solution softening in nickel-aluminum alloys induced by iron, manganese and chromium solute atoms, which cannot be explained by the current hardening theories. Quantum mechanical calculations revealed the development of a large electron-spin polarization when these solute atoms substitute for aluminum in nickel-aluminum alloys. The spin polarization results in a large magnetic moment that dilates the lattice parameter and strongly affects mechanical properties of nickel-aluminum alloys. The calculated values are unambiguously supported by EELS and polarized neutron diffraction. These studies have led to the discovery of a new concept in the design of strong and tough intermetallic and metallic alloys for advanced heat engines and energy conversion systems. This new principle is expected to appear in textbooks illustrating cross-fertilization between two disciplines which have had no connection.

Reference: C.T. Liu, et al., *Acta Materialia* 50, 3203-3210 (2002).

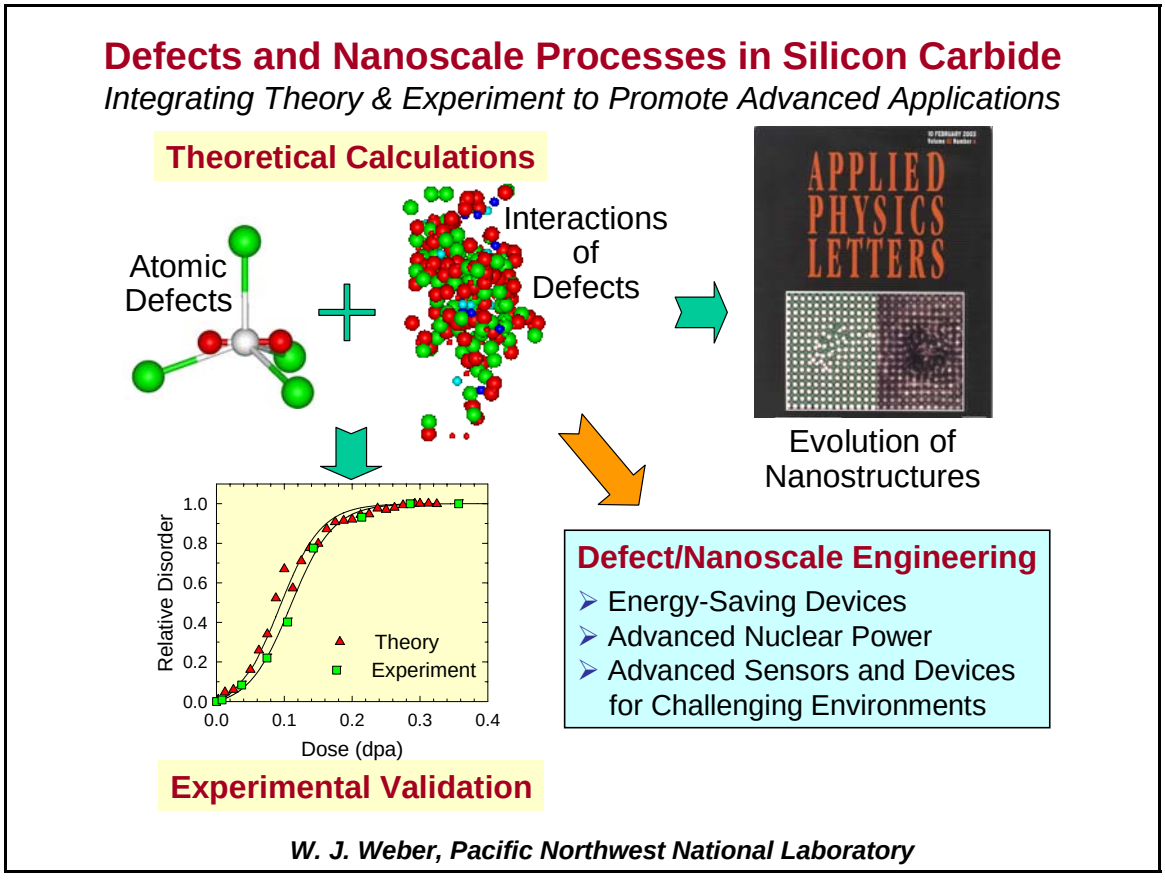


Silicon Carbide: Going Where Silicon-Based Technology Cannot Go

Investigator: W. J. Weber, Pacific Northwest National Laboratory

Major breakthroughs in understanding atomic defects and nanostructures in silicon carbide enable this semiconductor material to be used in a new generation of devices for severe environments where silicon-based devices cannot operate. This new understanding can be used to overcome materials degradation problems that hinder advanced device development. Atomistic computational methods have determined critical defect formation and diffusion properties and accurately predicted evolution of nanostructures, phase transformations, and changes in volume and mechanical properties. The excellent agreement between computational predictions and experimental measurements provides the scientific confidence to use the computational methods to predict properties and behavior under extreme conditions that cannot be tested in the laboratory and to use defect engineering to minimize degradation, enhance materials reliability, and design materials that allow the remarkable physical properties and biocompatibility of silicon carbide to be fully utilized for energy-saving devices, advanced optoelectronics, improved sensors, medical devices, advanced-energy components, and chemically-challenging environments.

References: F. Gao and W. J. Weber, *Appl. Phys. Lett*. 82, 913 (2003); Y. Zhang, W. J. Weber, W. Jiang, C. M. Wang, A. Hallén, and G. Possnert, *J. Appl. Phys*. *93 [4]:* 1954-1960 (2003). F. Gao and W. J. Weber, *Phys. Rev. B 66 [2]:* 024106, 1-10 (2002).



Atomic Scale Revelations of Brittle Fracture

Investigator: J. G. Swadener, M. I. Baskes, M. Nastasi, Los Alamos National Laboratory

A molecular dynamics study has revealed for the first time how fracture processes at the atomic scale affect bulk properties, such as dynamic fracture toughness and crack propagation rate. Using an interatomic potential derived from the modified embedded atom method, the atomistic calculations showed that at low speeds, silicon fractures via perfect cleavage on atomic planes, but at higher speeds, atomic lattice defects, uneven crack surfaces and phonon vibrations are produced leading to an increase in the energy consumed during fracture. This increased energy consumption reduces the energy that would otherwise be available to drive cracks to even higher propagation rates and limits the maximum crack propagation rate to significantly less than the theoretical maximum crack propagation rate. The results demonstrate that molecular dynamics can be used to accurately reproduce bulk experimental results, while simultaneously capturing the atomic level details of the fracture process. The added significance of this method is that it can be easily extended to other materials and incorporated into models of large dynamic systems.

Reference: *Phys. Rev. Lett.* 89, 85503 (2002).